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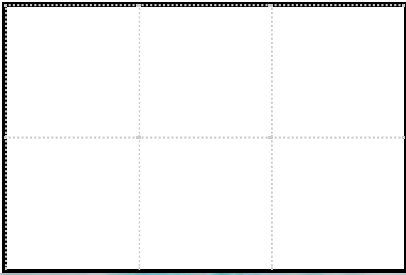
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WATER

'Portable Oasis' Extracts Water from Dry Desert Air

An ultraporous humidity sponge could provide 300 gallons of fresh water a day

By Steven Ashley on November 17, 2021

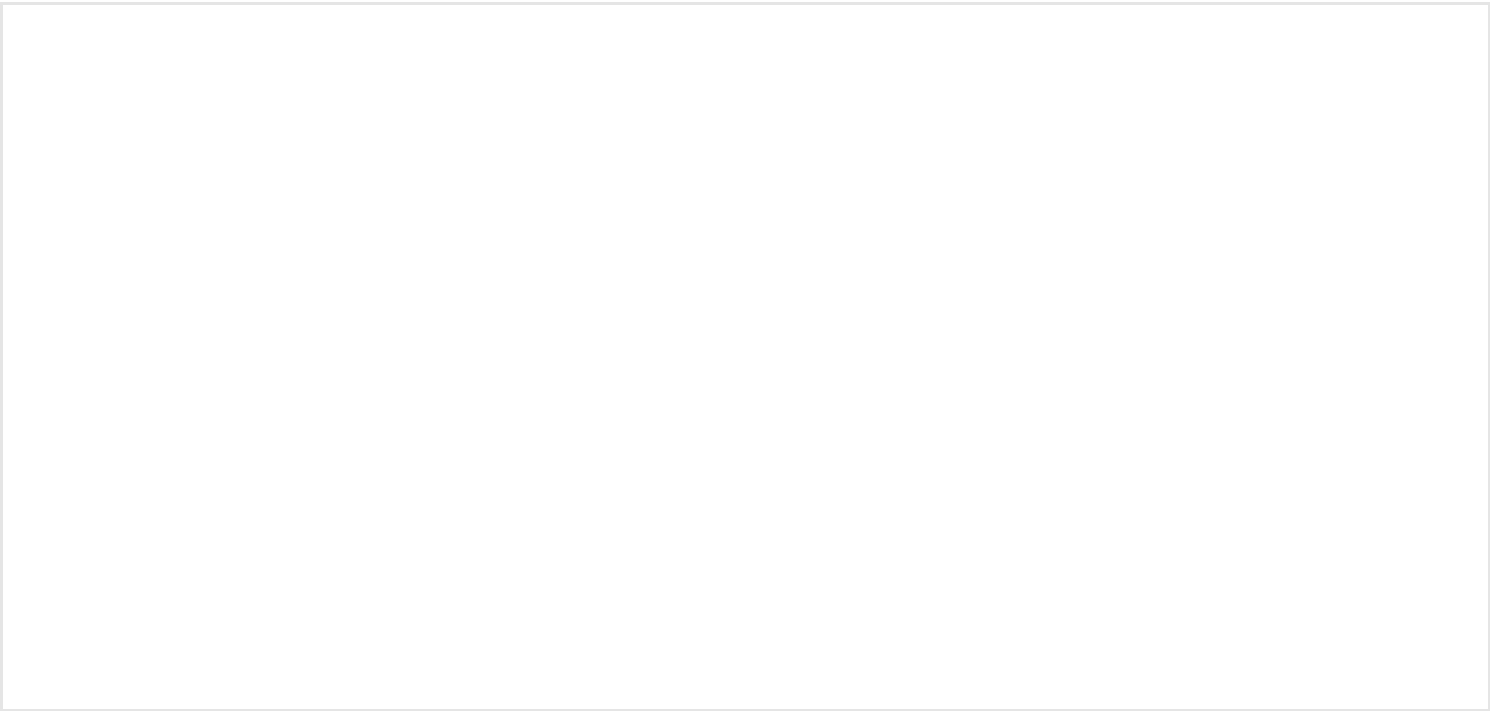


Credit: Xuanyu Han *Getty Images*

An ultraporous compound can extract water molecules from dry desert air, store them as tiny “icicles” and then release them as clean drinking water. A new study has shown this novel humidity sponge’s developers how it works in detail, taking it a step closer to practical applications. Along with government, industry and university partners, the researchers are working to turn their project into portable hydration systems capable of conjuring fresh water almost anywhere in an increasingly thirsty world.

The technology relies on an aluminum-based compound called MOF-303, one of more than 20,000 designer materials known as metal-organic frameworks, or MOFs. These substances are made up of both inorganic and organic molecules, which link together to form open lattice structures that resemble Tinkertoy stick-and-node play sets: Central “nodes” of metal ions bind to multiple organic “stick” molecules, producing a cagelike framework. The resulting porous crystal structure is so fully honeycombed with pockets that a chunk the size of a sugar cube can contain several football fields’ worth of internal surface area. These surfaces can attract and bind with many simple gas molecules such as methane, hydrogen and water, as well as more complex compounds, including pollutants and nerve gas agents. Thanks to their gas-grabbing abilities, MOFs are useful in a variety of practical applications, and MOF-303 is particularly good at squeezing traces of humidity from the air.

The specific mechanism underlying these superior water-extraction abilities has now been explained by an international team led by University of California, Berkeley, chemist Omar Yaghi. “We figured out which water comes first and the way it fills up, step by step,” he says. Yaghi’s team had previously developed MOF-303 specifically for water extraction and successfully demonstrated it in dry laboratory conditions and an Arizonan desert. In their new study, published last month in *Science*, they analyzed MOF-303 using precise x-ray diffraction measurements that determine a molecule’s structure by measuring the way reflected x-rays interfere with one another.



The experimental results matched theoretical predictions the researchers had made about MOF-303's behavior: The material's nanoscale pockets readily fill up with water vapor because the internal pore walls are "decorated" with sites that attract water molecules, Yaghi says. The first water molecules to arrive at such sites anchor themselves in place. These captured molecules rapidly form hydrogen bonds with other passing water molecules, seeding what Yaghi describes as dense, ambient-temperature ice crystals. Although they remain at air temperature, the molecules join together like they do in ice, filling the pores with solid water structures. "First the water molecules form isolated clusters, then chains of clusters, and finally a water network carpets the interior space," he explains. Once the MOF has filled its pores with these minuscule icicles, applying a little extra heat is enough to release the molecules as potable drinking water.

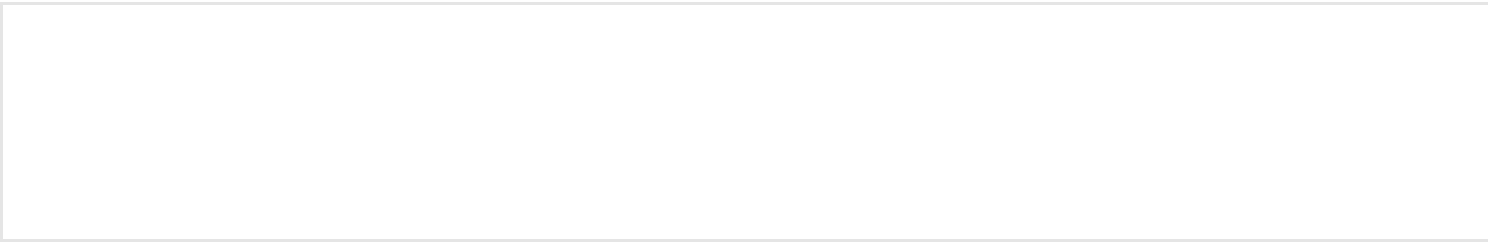
For researchers hoping to improve MOF performance, Yaghi's detailed description of the mechanism this material uses to capture water is important. "Once you know the mechanism, you know how to improve it," says Hong-Cai "Joe" Zhou, an organic

chemist at Texas A&M University, who works on MOFs and other porous materials and was not involved in the study. “It’s fantastic that they solved this problem.”

The new MOF-303 study is supported by the U.S. Defense Advanced Research Projects Agency’s Atmospheric Water Extraction program: a four-year research-and-development effort that aims to reduce the risks and logistic costs of transporting water supplies to troops in the field. Its goal is to replace current options such as shipped bottled water, desalination using reverse osmosis and fog-catching structures—each of which comes with its own problems. In the longer run, similar technology might help address growing water scarcity around the world.

If the project succeeds, says Blake Bextine, a program manager at DARPA, the new water-harvesting technology could mean that combat troops, disaster-relief teams and others in remote regions far from potable water sources may, in time, benefit from truck-borne “portable oasis” stations—pallet-size, self-contained hydration units weighing around 300 pounds. When connected to a diesel power generator to drive a fan and heater, Bextine says, a unit could reliably, efficiently and affordably produce at least 300 gallons a day of fresh water—enough to supply an Army-company-size group of 150 people. A prototype will undergo testing in mid-2022.

To develop water harvester devices using MOFs, Yaghi and his colleagues are working with a General Electric (GE) research-and-development team and two other university groups. GE, which received a \$5.4-million DARPA grant to serve as lead investigator of the project and to build the device, is modeling, designing and engineering it to make it as simple and efficient as possible. Meanwhile the university groups (one led by theoretical computational chemist Laura Gagliardi of the University of Chicago and the other by chemical engineer Grant Glover of the University of South Alabama) are using molecular simulations and precise experimental measurements to figure out how this material might capture even more water even more easily.



Although MOF-303 works extremely well already, Bextine says, it could be improved. “Not all the water adsorbs equally within the material,” he explains. “If you’re loading up the front sites first, as water molecules flow into the pocket, it can impede full uptake.” The process is a little like boarding an airliner: If everyone grabs the first seats up front, that slows access to the rear seats. But if the passengers can be persuaded to find a place farther back, the airliner cabin—or storage pores in the case of MOF-303—can fill up faster and more efficiently. As Gagliardi puts it, “The sites need to bind enough but not too much.”

Yaghi and his colleagues say they can achieve these Goldilocks-level binding sites by tweaking the types of organic molecules used as the “sticks” of the Tinkertoy structure. “Essentially, we can mix into the framework alternate linker units containing, say, oxygen or sulfur rather than nitrogen—but with the same geometry—to modulate the binding energy of the pocket walls and improve water uptake by 15 percent,” Yaghi says. “At the same time, we control the temperature of desorption, so you can still remove the water without a lot of heat.”

The new study is “a beautiful example,” Zhou says. And it shows that “understanding the detailed mechanisms at the atomic and molecular level should, in the future, help researchers find solutions in emerging biomedical applications—including smart drug delivery, nuclear magnetic imaging and phototherapy.” The insights gained from this research could also allow chemists to shape MOFs’ water-uptake behavior and potentially design even better humidity sponges. In the future, these materials might prove to be a lifeline for drought- or disaster-stricken people around the world.



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